

Renormalization-group approach to the metal-insulator transitions in $(\text{DCNQI})_2\text{M}$ (DCNQI is N, N' -dicyanoquinonediimine and $\text{M}=\text{Ag}, \text{Cu}$)

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Metal-insulator transitions and different ground-state phases in quasi-one-dimensional materials, $(R_1R_2\text{-DCNQI})_2\text{M}$ ($R_1=R_2=\text{CH}_3$, I and $\text{M}=\text{Ag}, \text{Cu}$), are studied with a renormalization-group method. We use one-dimensional continuum models with backward scatterings, umklapp processes and couplings with $2k_F$ and $4k_F$ phonons (not static lattice distortion). We take a quarter-filled band for $\text{M}=\text{Ag}$ and a sixth-filled band coupled with a third-filled band for $\text{M}=\text{Cu}$. Depending on electron-electron and electron-phonon coupling strengths, the ground-state phase becomes a Tomonaga-Luttinger liquid or a state with a gap(s). For $\text{M}=\text{Ag}$, there appear a spin-gap state with a dominant $2k_F$ charge-density-wave correlation, a Mott insulator with a dominant $4k_F$ charge-density-wave correlation, or a spin-Peierls state with different magnitudes of spin and charge gaps. Three-dimensionality is taken into account by cutting off the logarithmic singularity in either the particle-particle channel or the particle-hole channel. The difference between the ground-state phase of the $R_1=R_2=\text{CH}_3$ salt (spin-Peierls state) and that of the $R_1=R_2=\text{I}$ salt (antiferromagnetic state) is qualitatively explained by a difference in the cutoff energy in the particle-particle channel. For $\text{M}=\text{Cu}$, there appear a Mott insulator with a charge density wave of period 3 and a Peierls insulator with a charge density wave of period 6. The conditions for the experimentally observed, Mott insulator phase are strong correlation in the sixth-filled band, moderate electron-phonon couplings, and finite electron- $4k_F$ phonon coupling. Resistance is calculated as a function of temperature with a memory-function approximation in both cases above. It qualitatively reproduces the differences among the $\text{M}=\text{Ag}$ and $\text{M}=\text{Cu}$ cases as well as the $R_1=R_2=\text{CH}_3$ and $R_1=R_2=\text{I}$ cases.

I. INTRODUCTION

Quasi-one-dimensional materials, $(R_1R_2\text{-DCNQI})_2\text{M}$ ($\text{M}=\text{Ag}, \text{Cu}$), show various phases. For $\text{M}=\text{Cu}$, the hybridization of DCNQI π orbitals and Cu d orbitals causes intriguing transport [1] and magnetic [2] properties. The metal-insulator transition is accompanied by the formation of a charge density wave (CDW) of period 3. [2,3] The low-temperature phase is a Mott insulator, which is caused by strong correlation of d electrons in cooperation with electron-lattice coupling and cannot be described by a band picture. In fact, the spin susceptibility in the insulating state is enhanced over the temperature-independent Pauli-like paramagnetism seen in the metallic state. It has called forth theoretical studies, most of which have used mean fields [4] — the Hartree-Fock approximation and the mean field approximation for slave bosons. The $1/N$ correction to the latter explains the overall phase diagram rather well. The cooperative effect has been discussed on phenomenological grounds. [5] Here we take a different approach, which qualitatively reproduces exactly known, ground-state properties near the metal-insulator transition in one dimension.

For $\text{M}=\text{Ag}$, the Ag d level is far away from the Fermi energy so that the DCNQI π bands are quarter filled. In this sense, they are similar to $(\text{TMTTF})_2\text{X}$ and $(\text{TMTSF})_2\text{X}$ salts, which are also quarter-filled and show various phases. [6] In the latter, the $4k_F$ anion potential has been considered to produce the umklapp process [7] and then to cause the metal-insulator transition. [8] Such an extrinsic potential is absent in the $(R_1R_2\text{-DCNQI})_2\text{Ag}$ salts, but the metal-insulator transition occurs, accompanied by the formation of a $4k_F$ CDW for both of the $R_1=R_2=\text{CH}_3$ (denoted by DMe hereafter) and $R_1=R_2=\text{I}$ (denoted by DI hereafter) cases. [9] At low temperatures, $(\text{DMe-DCNQI})_2\text{Ag}$ becomes a spin-Peierls state, while $(\text{DI-DCNQI})_2\text{Ag}$ becomes an antiferromagnet. [10] Thus electron correlation in the π band also plays an essential role to determine the ground-state phases.

Electron correlation is essential in low dimensions. In pure one dimension, the Fermi liquid is unstable against any perturbation. When the perturbation is irrelevant in terms of a renormalization group, the excitation spectrum is gapless. Then the low-energy limit of the property is described by the Tomonaga-Luttinger liquid theory and characterized by power laws in the density of states and various correlation functions. [11,12] Otherwise, the spectrum has a gap so that some of the correlation functions decay exponentially. [13]

For the metallic $(\text{DMe-DCNQI})_2\text{Cu}$, the single-particle spectrum has been observed in photoemission experiments and described by a power law of the electron binding energy. [14] This suggests that the metallic phase is described by the Tomonaga-Luttinger liquid theory for low but not extremely low temperatures. The exponent is much larger

than the calculated one for the Hubbard model or the extended Hubbard model with on-site and nearest-neighbor repulsions only. However, it can be explained by long-range interactions. [15,16] The power-law holds up to the binding energy as large as 0.3 eV. This fact would also indicate a long-range interaction. [14] Recently, suppression of the interchain coherent hopping by such a large exponent in the single-particle spectrum is numerically investigated. [16]

In the insulator phase on the other hand, the Cu d electrons are almost localized so that good one-dimensionality is expected. Since the nesting is perfect and the tendency to an insulator phase is strong in one dimension when coupled with phonons, the metal-insulator transition must be explained at least in a purely one-dimensional model in order for it to occur in a quasi-one-dimensional real system. We then employ a purely one-dimensional model to study conditions for the observed Mott insulator phase with a gapless spin mode.

Meanwhile, (DCNQI)₂Ag salts are insulators for low temperatures. One-dimensionality is expected to be better than (DCNQI)₂Cu salts because the metal ion does not help the electron propagation perpendicular to the most conducting direction as in the Cu salt. In fact, the one-dimensional band structure has been evidenced by the polarized reflectance spectra on single crystals. [17] Thus the Tomonaga-Luttinger liquid theory would be a good starting point. Qualitative aspects of the experimental findings are in fact explained by considering the effects of electron- $2k_F$ phonon coupling, electron- $4k_F$ phonon coupling, and slight three-dimensionality on a one-dimensional continuum model.

In one dimension, a renormalization-group method based on the scaling law is very useful to study the effects of various perturbations. The Mott transition is caused by the umklapp process. The temperature and frequency dependence of the conductivity for commensurate and nearly commensurate fillings has been studied in detail [18] with the renormalization-group method combined with a memory-function approximation. [19] The Mott transition which occurs when the correlation strength is changed and that which occurs when the filling is changed have different physical properties, which are clarified for even and odd commensurabilities. [20] Meanwhile, the electron-phonon interaction produces the retarded attraction. Its effect has also been studied with the renormalization-group method. When it contributes to the forward scattering, the backward scattering, and the umklapp process, it enhances the pairing correlation, the formation of a spin gap, [21] and the formation of a charge gap, [22,23] respectively.

Here, we apply the method to more complex systems, which have couplings with $2k_F$ and $4k_F$ phonons with one or two bands at even or odd commensurability. We derive and numerically solve the lowest-order equations to learn which phase the Tomonaga-Luttinger liquid approaches as the energy scale is lowered. Although a precise description of the electronic states at strong-coupling fixed points is beyond the scope of the present method, it indicates whether each excitation spectrum has a gap or not so that the ground-state phases can be classified accordingly. Such procedure reproduces qualitative tendency to the strong-coupling phases for nearly-half-filled electron-phonon systems [22,23] and for a two-coupled-chain system. [24] The present paper also follows the procedure.

To compare with experimental results, it would be necessary to take weak three-dimensionality into account. The scaling law and the consequent power-law behavior of various quantities in one dimension result from the interference of the logarithmic singularity in the $2k_F$ particle-hole channel with that in the particle-particle channel. The contributions from the corresponding lowest-order bubble diagrams are different in signs only. Quasi-one-dimensionality would be simulated by different cutoff energies for the two logarithmic singularities and the consequent imbalance between the two channels. [7] In the M=Ag case, we find that the differences between the $R_1=R_2=\text{CH}_3$ salt of the spin-Peierls ground state and the $R_1=R_2=\text{I}$ salt of the antiferromagnetic ground state are qualitatively explained by a difference in the cutoff energy in the particle-particle channel.

In the M=Cu case, the two-band feature is essential. The interference between electron-phonon couplings, backward scatterings and umklapp processes is much more complicated in the two-band case than in the single-band case. The phonons with momenta near $2\pi/3$ are responsible for the $4k_F$ scattering in the sixth-filled band and for the $2k_F$ and $4k_F$ scatterings in the third-filled band, while the phonons with momenta near $\pi/3$ are responsible for the $2k_F$ scattering in the sixth-filled band. Different combinations of the above scatterings lead to different backward scattering or umklapp processes, opening charge gaps in both of the sixth-filled and third-filled bands. The insulator phase can have a spin gap only in the third-filled band (Mott insulator) or spin gaps in both bands (Peierls insulator). The former phase is realized when the sixth-filled band (*i.e.*, π - d hybrid band [25]) has strong correlation and the electron- $2k_F$ phonon coupling is moderate. The electron- $4k_F$ phonon coupling is necessary here, though it may not be strong. The latter phase is realized when the electron- $2k_F$ phonon coupling is strong.

To study how the behavior of resistance depends on the commensurability and model parameters, we use a memory-function approximation. For M=Ag, the renormalization-group method qualitatively reproduces the difference between the DMe and DI cases. For M=Cu, the behavior of the resistance above the transition temperature is less sensitive to changes in correlation strengths than in the quarter-filled case. Experimentally, the transition is of first order due to the third-order commensurability energy, [26] and it needs three-dimensionality in phonons, which is beyond the scope of the present study.

This paper is organized as follows: Sec. II introduces bosonized models based on one-dimensional continuum models with backward scatterings, umklapp processes, and couplings with $2k_F$ and $4k_F$ phonons. Sec. III outlines the

derivation of renormalization group equations, clarifying how different electron-phonon couplings effectively produce different backward scattering or umklapp processes and how they open gaps in different channels. Secs. IV and V show phase diagrams for different parameters and resistance as a function of temperature for M=Ag and M=Cu, respectively, to compare them with the experimental results. Sec. VI summarizes the present work. Part of the results presented in this paper were reported briefly elsewhere. [27]

II. MODELS

We consider a continuum model in which the noninteracting part is a Tomonaga-Luttinger liquid extended to include the spin (denoted by subscript σ) and charge (denoted by subscript ρ) degrees of freedom,

$$H_0 = \sum_{\nu=\sigma,\rho} \int \frac{dx}{2\pi} \left[u_\nu K_\nu (\partial_x \theta_\nu(x))^2 + \frac{u_\nu}{K_\nu} (\partial_x \phi_\nu(x))^2 \right], \quad (2.1)$$

where fields $\phi_\nu(x)$ and $(1/\pi)\partial_x \theta_\nu(x)$ are conjugate, u_ν and K_ν are the velocity and the correlation exponent of the ν channel, respectively, which are standard notations and described in detail in the previous paper. [22] For M=Ag, we consider a quarter-filled band. For M=Cu, we take two bands and distinguish them by subscripts: A for the sixth-filled band; B for the third-filled band. Then, the noninteracting part is the sum of H_{A0} and H_{B0} , in which the summation is performed over $\nu=A\sigma$, $A\rho$ and $\nu=B\sigma$, $B\rho$, respectively. It is noted that $H_{(C)0}$ ($C = A, B$) [*i.e.*, H_0 , H_{A0} , or H_{B0}] contains the (one-electron) kinetic part and the forward scattering. For M=Cu, we consider, for simplicity, the regime where the Fermi velocity in the A band and that in the B band do not differ so much. Since we do not expect that the difference in the Fermi velocities affects the scenario to the metal-insulator transition, we use the averaged Fermi velocity, v_F . For later convenience, we define $X_{(C)\sigma} = 2(1 - K_{(C)\sigma}^{-1}) \simeq g_{(C)1}/(\pi v_F)$ and $X_{(C)\rho} = 2(1 - K_{(C)\rho}^{-1}) \simeq (g_{(C)1} - 2g_{(C)2})/(\pi v_F)$ for $C = A, B$, where $g_{(C)1}$ and $g_{(C)2}$ are the backward and forward scattering strengths (in the C band), respectively. In terms of the single-band extended Hubbard model with on-site (U) and nearest-neighbor (V) repulsions, $X_\sigma = U/(\pi v_F)$, $X_\rho = -(U + 4V)/(\pi v_F)$ for quarter filling, $X_{A\sigma} = (U + V)/(\pi v_F)$, $X_{A\rho} = -(U + 3V)/(\pi v_F)$ for sixth filling, and $X_{B\sigma} = (U - V)/(\pi v_F)$, $X_{B\rho} = -(U + 5V)/(\pi v_F)$ for third filling.

A. Electron-electron interactions

A backward scattering between antiparallel spins of strength $Y_{(C)\sigma} = g_{(C)1}/(\pi v_F)$,

$$H_{(C)\sigma} = Y_{(C)\sigma} \pi v_F \sum_s \int dx \psi_{(C)1,s}^\dagger(x) \psi_{(C)2,-s}^\dagger(x) \psi_{(C)1,-s}(x) \psi_{(C)2,s}(x), \quad (2.2)$$

where $\psi_{(C)1,s}$ and $\psi_{(C)2,s}$ are right- and left-going electrons with spin s (in the C band), is written with the phase field as

$$H_{(C)\sigma} = \frac{Y_{(C)\sigma} v_F}{2\pi\alpha^2} \int dx \cos \left[2\sqrt{2}\phi_{(C)\sigma}(x) \right], \quad (2.3)$$

where α is a cutoff parameter of the order of the inverse of the Fermi wave number.

To study metal-insulator transition, we need to include high-order electron-electron scattering processes, which are to be produced in the renormalization process when electron-phonon interactions are included. In the $1/m$ -filled band, the Fermi wave number is π/m so that the umklapp process is written as

$$H_{U,m}[\phi_\rho, \phi_\sigma; Y_\rho] \propto Y_\rho v_F a^{m-2} \int dx \left[\sum_s \psi_{1,s}^\dagger(x) \psi_{2,s}(x) \right]^m + \text{h.c.}, \quad (2.4)$$

where Y_ρ is a coupling strength such that the prefactor appears simple in the phase-field representation, a is of the order of the lattice spacing and set to be α , and the power should be understood as point-split hereafter. With the phase-field operators, it is rewritten as

$$H_{U,m}[\phi_\rho, \phi_\sigma; Y_\rho] = \begin{cases} (Y_\rho v_F)/(2\pi\alpha^2) \int dx \cos[m\sqrt{2}\phi_\rho(x)] & \text{for even } m, \\ (Y_\rho v_F)/(\sqrt{2}\pi\alpha^2) \int dx \cos[m\sqrt{2}\phi_\rho(x)] \cos[\sqrt{2}\phi_\sigma(x)] & \text{for odd } m, \end{cases} \quad (2.5)$$

where and hereafter less relevant terms are neglected. Thus, we have $H_\rho = H_{U,4}[\phi_\rho; Y_\rho]$ for the quarter-filled band, $H_{A\rho} = H_{U,6}[\phi_{A\rho}; Y_{A\rho}]$ for the sixth-filled band, $H_{B\rho\sigma} = H_{U,3}[\phi_{B\rho}, \phi_{B\sigma}; Y_{B\rho\sigma}]$ and $H_{B\rho} = H_{U,6}[\phi_{B\rho}; Y_{B\rho}]$ (which is included though less relevant than $H_{B\rho\sigma}$) for the third-filled band. In terms of the extended Hubbard model, $Y_\rho = 3U^3/(16\pi^3 t^2 v_F) = 3Y_\sigma^3/8$, *etc.* As m increases, the effect of $H_{U,m}$ becomes weak on opening a gap, as explicitly shown in the renormalization-group equations later. Note that, for odd m , the umklapp process involves the spin degrees of freedom: [20] when the umklapp process flows to a strong-coupling fixed point, there are gaps in both the charge and spin excitations. In such a case, soliton excitations carry both charge and spin in contrast to the case with even m .

In addition, there are interband scattering processes for $M=\text{Cu}$. The most relevant backward scattering is written as

$$H_{AB\rho\sigma} = (Y_{AB\rho\sigma}\pi^2 v_F a / \sqrt{2}) \int dx \left[\sum_s \psi_{A1,s}^\dagger(x) \psi_{A2,s}(x) \right]^2 \left[\sum_s \psi_{B2,s}^\dagger(x) \psi_{B1,s}(x) \right] + \text{h.c.} , \quad (2.6)$$

where $Y_{AB\rho\sigma}$ is the coupling strength. It is rewritten as

$$H_{AB\rho\sigma} = \frac{Y_{AB\rho\sigma} v_F}{\sqrt{2}\pi\alpha^2} \int dx \cos \left[2\sqrt{2}\phi_{A\rho}(x) - \sqrt{2}\phi_{B\rho}(x) \right] \cos \left[\sqrt{2}\phi_{B\sigma}(x) \right] , \quad (2.7)$$

which involves the charge degrees of freedom in the A band and both the charge and the spin degrees of freedom in the B band. The scaling dimension is the lowest (in the noninteracting limit) among the perturbations involving the charge degrees of freedom. So, this is the most likely candidate which causes a metal-insulator transition. When this backward scattering (not umklapp process) flows to a strong-coupling fixed point, there are at least three gaps in the corresponding channels. Meanwhile, the most relevant umklapp process is written as

$$H_{AB\rho} = Y_{AB\rho\sigma}\pi^3 v_F a^2 \int dx \left[\sum_s \psi_{A1,s}^\dagger(x) \psi_{A2,s}(x) \right]^2 \left[\sum_s \psi_{B1,s}^\dagger(x) \psi_{B2,s}(x) \right]^2 + \text{h.c.} , \quad (2.8)$$

where $Y_{AB\rho}$ is the coupling strength. It is rewritten as

$$H_{AB\rho} = \frac{Y_{AB\rho} v_F}{2\pi\alpha^2} \int dx \cos \left[2\sqrt{2}\phi_{A\rho}(x) + 2\sqrt{2}\phi_{B\rho}(x) \right] , \quad (2.9)$$

which involves the charge degrees of freedom in both bands but does not involve the spin degrees of freedom.

B. Electron-phonon interactions

As to phonons, we need to consider those with momenta near $2k_F$ and those with momenta near $4k_F$. Because we are not interested in superconductivity here, we do not consider phonons with momenta near $0k_F$, though the extension is straightforward. [22,27] The wave numbers $\mu=2k_F$, $4k_F$ are $\mu=\pi/2$, π for $m=4$, $\mu=\pi/3$, $2\pi/3$ for $m=6$, and $\mu=2\pi/3$, $4\pi/3(=-2\pi/3)$ for $m=3$. The corresponding phonon fields and their conjugate momenta are denoted by $\phi_\mu(x)$ and $\Pi_\mu(x)$, respectively. The fields $\phi_\pi(x)$ and $\Pi_\pi(x)$ are real, and the others are complex. The phonon parts of the models are written as

$$H_\mu = \int dx \left[\Pi_\mu(x) \Pi_{-\mu}(x) + \omega_\mu^2 \phi_\mu(x) \phi_{-\mu}(x) \right] \quad (2.10)$$

for the complex fields ($\mu \neq \pi$) and

$$H_\pi = \frac{1}{2} \int dx \left[\Pi_\pi^2(x) + \omega_\pi^2 \phi_\pi^2(x) \right] \quad (2.11)$$

for the real fields, where ω_μ and ω_π are the corresponding phonon frequencies.

Electron- $2k_F$ phonon coupling is generally written as

$$H_{1,(C),\mu} = \sqrt{\pi v_F \omega_\mu} y_{(C)1} \sum_s \int dx \psi_{(C)2s}^\dagger(x) \psi_{(C)1s}(x) \phi_\mu(x) + \text{h.c.} , \quad (2.12)$$

where $y_{(C)1}$ is the strength of the $2k_F$ scattering (in the C band) by a phonon. It is rewritten as

$$H_{1,(C),\mu} = \frac{\sqrt{v_F}\omega_\mu y_{(C)1}}{\sqrt{\pi}\alpha} \int dx \cos\left[\sqrt{2}\phi_{(C)\sigma}(x)\right] e^{-i\sqrt{2}\phi_{(C)\rho}(x)} \phi_\mu(x) + \text{h.c.} \quad (2.13)$$

For the quarter-filled band, for example, the coupling strength and the phonon frequencies are given by $y_1 = \beta/\sqrt{\pi v_F K}$ and $\omega_{\pi/2} = \omega_\pi = \sqrt{K/M}$ for the Holstein coupling, [28] $\sum_i (\beta q_i n_i + \frac{K}{2} q_i^2 + \frac{1}{2M} p_i^2)$, with coupling strength β , spring constant K , ionic mass M , electron density n_i at site i , lattice displacement q_i and its conjugate momentum p_i , and by $y_1 = 2i\alpha_S/\sqrt{\pi v_F K}$ and $\sqrt{2}\omega_{\pi/2} = \omega_\pi = 2\sqrt{K/M}$ for the SSH coupling, [29] $\sum_i \left[\alpha_S q_{i,i+1} \sum_s (c_{i,s}^\dagger c_{i+1,s} + \text{h.c.}) + \frac{K}{2} q_{i,i+1}^2 + \frac{1}{2M} p_i^2 \right]$, with coupling strength α_S , $q_{i,i+1} = q_{i+1} - q_i$, $c_{i,s}$ annihilating an electron with spin s at site i , and other parameters as defined above.

Electron- $4k_F$ phonon coupling is generally written as

$$H_{3,(C),\mu} = -\sqrt{2\pi^3 v_F \omega_\mu y_{(C)3}} \sum_{s,s'} a \int dx \psi_{(C)2s}^\dagger(x) \psi_{(C)2s'}^\dagger(x) \psi_{(C)1s'}(x) \psi_{(C)1s}(x) \phi_\mu(x) + \text{h.c.}, \quad (2.14)$$

where $y_{(C)3}$ is the strength of the $4k_F$ scattering (in the C band) by a phonon. It is rewritten as

$$H_{3,(C),\mu} = -\frac{\sqrt{v_F}\omega_\mu y_{(C)3}}{\sqrt{2\pi}\alpha} \int dx e^{-i2\sqrt{2}\phi_{(C)\rho}(x)} \phi_\mu(x) + \text{h.c.} \quad (2.15)$$

For the quarter-filled band, for example, the coupling strength is given by $y_3 = \beta'/\sqrt{8\pi^3 v_F K}$ for the electron-electron-phonon coupling, $\sum_i (U - \beta' q_i n_{i\uparrow} n_{i\downarrow})$, with on-site repulsion U , coefficient β' of its modulation by lattice displacement q_i , electron density n_{is} with spin s at site i , and by $y_3 = i\alpha'/\sqrt{2\pi^3 v_F K}$ for the electron-electron-phonon coupling, $\sum_{i,s,s'} (V - \alpha' q_{i,i+1}) n_{is} n_{i+1s'}$, with nearest-neighbor repulsion V , coefficient α' of its modulation by lattice displacement $q_{i,i+1}$.

The phonon fields are bilinear, so that they can be integrated out completely to produce effective retarded interactions, [22] which are lengthy and not shown here. In the $\omega_\mu \rightarrow \infty$ limit, the electron-phonon interactions do nothing but shift the parameters, $X_{(C)\sigma} \rightarrow X_{(C)\sigma} - |y_{(C)1}|^2$, $Y_{(C)\sigma} \rightarrow Y_{(C)\sigma} - |y_{(C)1}|^2$, $X_{(C)\rho} \rightarrow X_{(C)\rho} - |y_{(C)1}|^2 - 4|y_{(C)3}|^2$, $Y_\rho \rightarrow Y_\rho - (y_3^2 + y_3^{*2})/2$, $Y_{B\rho\sigma} \rightarrow Y_{B\rho\sigma} + (y_{B1}y_{B3} + y_{B1}^*y_{B3}^*)$, $Y_{AB\rho\sigma} \rightarrow Y_{AB\rho\sigma} + (y_{B1}y_{A3}^* + y_{B1}^*y_{A3})$, and $Y_{AB\rho} \rightarrow Y_{AB\rho} - (y_{A3}y_{B3} + y_{A3}^*y_{B3}^*)$. Below we take the Hamiltonian

$$H = H_0 + H_\sigma + H_\rho + H_{\pi/2} + H_\pi + H_{1,\pi/2} + H_{3,\pi} \quad (2.16)$$

for M=Ag with a quarter-filled band, and

$$H = \sum_{C=A,B} (H_{C0} + H_{C\sigma} + H_{C\rho}) + H_{B\rho\sigma} + H_{AB\rho\sigma} + H_{AB\rho} + H_{\pi/3} + H_{2\pi/3} + H_{1,A,\pi/3} + H_{1,B,2\pi/3} + H_{3,A,2\pi/3} + H_{3,B,-2\pi/3} \quad (2.17)$$

for M=Cu with coupled sixth- and third-filled bands.

III. RENORMALIZATION EQUATIONS

We have derived the equations following the previous study. [22] We will give an outline for discussions later. The present one-dimensional quantum-mechanical system is mapped to a two-dimensional classical system where Burgers vectors interact with one another. The correlation function

$$\langle T_\tau e^{i\sqrt{2}\phi_{(C)\nu}(x,\tau)} e^{-i\sqrt{2}\phi_{(C)\nu}(0,0)} \rangle \quad (C = A, B, \quad \nu = \sigma, \rho) \quad (3.1)$$

is perturbationally developed and successively integrated by changing the length scale little by little. In this process, there are two possibilities for the fate of Burgers vectors: a pair of neutral Burgers vectors are annihilated in the larger length scale; and a pair of non-neutral Burgers vectors are combined to produce another Burgers vector. The latter is important since it causes various interference effects. [22,23] By comparing the correlation functions in successive length scales, we find relations between the effective parameters in the larger energy (*i.e.*, smaller length) scale and those in the smaller energy (*i.e.*, larger length) scale, which are described by differential equations (called renormalization-group equations) shown below.

A. Quarter-filled band

The combinations for the non-neutral Burgers vectors in the renormalization process are (y_1, y_1^*, Y_σ) , (y_3, y_3, Y_ρ) , and (y_3^*, y_3^*, Y_ρ) , where (a, b, c) means that any two of them are combined to produce the complex conjugate of the third. In order to make a comparison with the half-filled case easier, we use the notation similar to that in the previous study, [22] $Y_1 = |y_1|^2$, $Y_3 = |y_3|^2$, and a form factor $f = (y_3^2 + y_3^{*2})/(2Y_3)$ which satisfies $-1 < f < 1$. Below we mark the contributions from the particle-particle channel by $J_\eta(l)$ and those from the $2k_F$ particle-hole channel by $J_\kappa(l)$, which are useful to study a three-dimensionality effect later. Then, we finally have

$$dX_\sigma(l)/dl = -J_\eta(l) [X_\sigma(l) - X_\rho(l)] X_\sigma(l)/2 - J_\kappa(l) [X_\sigma(l) + X_\rho(l)] X_\sigma(l)/2 - Y_1(l) D_{\pi/2}(l), \quad (3.2)$$

$$dX_\rho(l)/dl = J_\eta(l) [3X_\sigma^2(l) + X_\rho^2(l)]/4 - J_\kappa(l) \{ [3X_\sigma^2(l) + X_\rho^2(l)]/4 + 4Y_\rho^2(l) \} - Y_1(l) D_{\pi/2}(l) - 4Y_3(l) D_\pi(l), \quad (3.3)$$

$$dY_\rho(l)/dl = J_\kappa(l) [2 - 8K_\rho(l)] Y_\rho(l) - fY_3(l) D_\pi(l), \quad (3.4)$$

$$dY_1(l)/dl = J_\kappa(l) [2 - K_\sigma(l) - K_\rho(l) - X_\sigma(l)] Y_1(l), \quad (3.5)$$

$$dY_3(l)/dl = J_\kappa(l) [2 - 4K_\rho(l) - fY_\rho(l)] Y_3(l), \quad (3.6)$$

where $l = \ln[E_F/E]$, $E(l)$ is a cutoff energy [$E(0) = E_F$], $K_\nu(l) = (1 - X_\nu(l)/2)^{-1}$, $D_\mu(l)$ is the phonon propagator defined by $D_\mu(l) = [\omega_\mu/E(l)] \exp[-\omega_\mu/E(l)]$. We have used the relation $X_\sigma(l) = Y_\sigma(l)$ due to the spin-rotational symmetry and omitted the equations for $u_\nu(l)$ which does not couple with the above equations in the present, lowest order. Initial conditions at $l = 0$ are determined by treating the effective retarded interactions carefully. [22] For $X_\sigma(0)$, $X_\rho(0)$, and $Y_\rho(0)$, only the phonon propagator is integrated from $-\infty$ to 0 with the fixed prefactor: $X_\sigma(0) = X_\sigma - Y_1 (1 - e^{-\omega_{\pi/2}/E_F})$, for example.

The reason why X_σ does not renormalize $X_\sigma(0)$ or why Y_1 is not renormalized at $l < 0$ in this example has been already discussed. [22] This correctly reproduces the antiadiabatic limit shown below (2.15).

In real materials, slight three-dimensionality would manifest itself at very low temperatures where the electron transport in the perpendicular direction becomes coherent. The renormalization-group method would not be justified deep in the anisotropic three-dimensional regime, where the scaling law no longer holds. However, the scaling law would deteriorate little by little as that regime is approached from above. Then we can see at least how the renormalization flow is deflected and which phase it tends to approach within the present method. The scaling law in one dimension results from the interference of the $2k_F$ particle-hole channel with the particle-particle channel. The corresponding lowest-order bubble diagrams are logarithmically divergent and have coefficients of equal magnitudes and different signs. Such interference disappears in higher dimensions because the Fermi surface does not consist of a finite number of points any more. Though the distortion of the Fermi surface removes the logarithmic singularity in the particle-hole diagram unless the nesting is perfect, the particle-particle channel generally becomes less important for repulsive interactions when only the particle-particle diagrams are summed infinitely. It is natural to regard quasi-one-dimensionality as causing imbalance between the two channels as the most important effect among all. [7] It is realized by different cutoff energies for the two logarithmic diagrams.

It should be noted that the renormalization-group equations derived from the bosonized model and the mapping to a two-dimensional classical system and those derived directly from the original fermion model are equivalent. [11] Renormalization of the velocities and detailed forms of cutoff functions if any (*e.g.*, one due to a misfit parameter) are generally different, but they are not essential. Deriving the renormalization equations again in the second method, we can distinguish the contributions from the particle-particle channel and the contributions from the $2k_F$ particle-hole channel, as already shown above. Then we can cut off either the particle-particle channel by the function $J_\eta(l)$ (determined below) or the $2k_F$ particle-hole channel by the function $J_\kappa(l)$. Assuming that the logarithm $\ln(E_F/E)$ is replaced by $\ln[E_F^2/(E^2 + \gamma^2 E_F^2)]/2$ ($\gamma = \eta, \kappa$) in the perturbation expansions, we obtain

$$J_\gamma(l) = (d/dl) \ln [E_F^2/(E^2(l) + \gamma^2 E_F^2)]/2 = (1 + \gamma^2 e^{2l})^{-1}, \quad (3.7)$$

which satisfies $J_0(l) = 1$, $J_{\gamma \neq 0}(l) \ll 1$ for $l \gg -\ln \gamma$ (*i.e.*, $E \ll \gamma E_F$), and $J_{\gamma \neq 0}(l) \rightarrow 0$ as $l \rightarrow \infty$.

The temperature dependence of the resistance shows how the system approaches the insulating/metallic ground state. It is a useful property to characterize the metal-insulator transition, and also a good indicator for the quality of theoretical approaches. Since we perform perturbative calculations above, we perform the perturbative expansion

for the conductivity following the study for commensurate and nearly commensurate fillings [18] with a memory-function formalism. [19] The conductivity is given by $\sigma(\omega) = (i2u_\rho K_\rho/\pi)[\omega + M(\omega)]^{-1}$, where the memory function $M(\omega)$ is defined by $M(\omega) = \omega \langle j; j \rangle_\omega / (\langle j; j \rangle_0 - \langle j; j \rangle_\omega)$ and $\langle j; j \rangle_\omega$ is the retarded correlation function of the current operator, $j(x) = \sqrt{2}u_\rho K_\rho \partial_x \theta_\rho(x)/\pi$. The lowest-order term in the perturbative expansion for $M(\omega)$ is $M(\omega) \simeq (\langle F; F \rangle_\omega^0 - \langle F; F \rangle_0^0) / (-\omega \langle j; j \rangle_0)$, where F is defined by $F = [j, H]$ and $\langle F; F \rangle_\omega^0$ stands for the retarded correlation function of the operator F at frequency ω computed in the absence of perturbations. Later we consider a temperature range below the phonon frequencies, where electron-phonon interactions are integrated out. The calculation of $\langle F; F \rangle_\omega^0$ is straightforward. Taking the $\omega \rightarrow 0$ limit, we finally have, for the resistance $R(T) = 1/\sigma(\omega = 0, T)$ at finite temperature T ,

$$R(T) \propto Y_\rho^2(T)TB^2[4K_\rho(T), 1 - 8K_\rho(T)]\cos^2[4\pi K_\rho(T)] , \quad (3.8)$$

where $B(x)$ is the beta function and $Y_\rho(T)$ denotes $Y_\rho[l = \ln(E_F/T)]$, *etc.* If we neglect the temperature dependence of K_ρ in the equation for Y_ρ (and for $\kappa = 0$), which would be valid only in the weak-coupling limit, $R(T) \propto Y_\rho^2 T^{16K_\rho-3}$. [18]

B. Coupled sixth- and third-filled bands

The combinations for the non-neutral Burgers vectors in the renormalization process are now $(y_{A3}, y_{B1}^*, Y_{AB\rho\sigma})$, $(y_{A3}, y_{B3}, Y_{AB\rho})$, $(y_{B1}, y_{B3}, Y_{B\rho\sigma})$, $(Y_{AB\rho\sigma}, Y_{AB\rho}, Y_{B\rho\sigma})$, $(Y_{AB\rho\sigma}, Y_{AB\rho\sigma}, Y_{B\sigma})$, $(Y_{B\rho\sigma}, Y_{B\rho\sigma}, Y_{B\sigma})$, $(Y_{B\rho\sigma}, Y_{B\rho\sigma}, Y_{B\rho})$, $(y_{A1}, y_{A1}^*, Y_{A\sigma})$, and $(y_{B1}, y_{B1}^*, Y_{B\sigma})$. When (a, b, c) is possible, (a^*, b^*, c^*) is also possible but it is not listed above because it is trivial. Note that y 's are complex parameters, while Y 's are real parameters. Finally, we have

$$dX_{A\sigma}(l)/dl = -X_{A\sigma}^2(l) - |y_{A1}(l)|^2 D_{\pi/3}(l) , \quad (3.9)$$

$$dX_{A\rho}(l)/dl = -Y_{AB\rho\sigma}^2(l) - Y_{AB\rho}^2(l) - 9Y_{A\rho}^2(l) - |y_{A1}(l)|^2 D_{\pi/3}(l) - 4|y_{A3}(l)|^2 D_{2\pi/3}(l) , \quad (3.10)$$

$$dX_{B\sigma}(l)/dl = -X_{B\sigma}^2(l) - \frac{1}{4}Y_{AB\rho\sigma}^2(l) - \frac{1}{4}Y_{B\rho\sigma}^2(l) - |y_{B1}(l)|^2 D_{2\pi/3}(l) , \quad (3.11)$$

$$dX_{B\rho}(l)/dl = -\frac{1}{4}Y_{AB\rho\sigma}^2(l) - Y_{AB\rho}^2(l) - \frac{9}{4}Y_{B\rho\sigma}^2(l) - 9Y_{B\rho}^2(l) - [|y_{B1}(l)|^2 + 4|y_{B3}(l)|^2] D_{2\pi/3}(l) , \quad (3.12)$$

$$dy_{A1}(l)/dl = \left\{ 1 - \frac{1}{2}[K_{A\sigma}(l) + K_{A\rho}(l) + X_{A\sigma}(l)] \right\} y_{A1}(l) , \quad (3.13)$$

$$dy_{A3}(l)/dl = [1 - 2K_{A\rho}(l)] y_{A3}(l) + \frac{1}{2}Y_{AB\rho\sigma}(l)y_{B1}(l) - \frac{1}{2}Y_{AB\rho}(l)y_{B3}^*(l) , \quad (3.14)$$

$$dy_{B1}(l)/dl = \left\{ 1 - \frac{1}{2}[K_{B\sigma}(l) + K_{B\rho}(l) + X_{B\sigma}(l)] \right\} y_{B1}(l) + \frac{1}{2}Y_{AB\rho\sigma}(l)y_{A3}(l) + \frac{1}{2}Y_{B\rho\sigma}(l)y_{B3}^*(l) , \quad (3.15)$$

$$dy_{B3}(l)/dl = [1 - 2K_{B\rho}(l)] y_{B3}(l) - \frac{1}{2}Y_{AB\rho}(l)y_{A3}^*(l) + \frac{1}{2}Y_{B\rho\sigma}(l)y_{B1}^*(l) , \quad (3.16)$$

$$\begin{aligned} dY_{AB\rho\sigma}(l)/dl &= \left\{ 2 - \frac{1}{2}[4K_{A\rho}(l) + K_{B\sigma}(l) + K_{B\rho}(l) + X_{B\sigma}(l)] \right\} Y_{AB\rho\sigma}(l) \\ &\quad - \frac{1}{2}Y_{AB\rho}(l)Y_{B\rho\sigma}(l) + [y_{B1}(l)y_{A3}^*(l) + y_{B1}^*(l)y_{A3}(l)] D_{2\pi/3}(l) , \end{aligned} \quad (3.17)$$

$$\begin{aligned} dY_{AB\rho}(l)/dl &= \{ 2 - 2[K_{A\rho}(l) + K_{B\rho}(l)] \} Y_{AB\rho}(l) \\ &\quad - \frac{1}{2}Y_{AB\rho\sigma}(l)Y_{B\rho\sigma}(l) - [y_{A3}(l)y_{B3}(l) + y_{A3}^*(l)y_{B3}^*(l)] D_{2\pi/3}(l) , \end{aligned} \quad (3.18)$$

$$dY_{B\rho\sigma}(l)/dl = \left\{ 2 - \frac{1}{2} [K_{B\sigma}(l) + 9K_{B\rho}(l) + X_{B\sigma}(l) + Y_{B\rho}(l)] \right\} Y_{B\rho\sigma}(l) - \frac{1}{2} Y_{AB\rho\sigma}(l) Y_{AB\rho}(l) + [y_{B1}(l) y_{B3}(l) + y_{B1}^*(l) y_{B3}^*(l)] D_{2\pi/3}(l), \quad (3.19)$$

$$dY_{A\rho}(l)/dl = [2 - 18K_{A\rho}(l)] Y_{A\rho}(l), \quad (3.20)$$

$$dY_{B\rho}(l)/dl = [2 - 18K_{B\rho}(l)] Y_{B\rho}(l) - \frac{1}{4} Y_{B\rho\sigma}^2(l), \quad (3.21)$$

where the cutoff energy and the phonon propagators are defined as before, $X_{C\sigma}(l) = Y_{C\sigma}(l)$ ($C = A, B$) has been used. Initial conditions at $l = 0$ are also determined as before.

For the present system, the resistance $R(T)$ in a temperature range below the phonon frequencies is given by

$$\begin{aligned} R(T) \propto & 5Y_{AB\rho\sigma}^2(T) T \cos^2 [\{4K_{A\rho}(T) + K_{B\rho}(T) + K_{B\sigma}(T)\} \pi/4] \\ & \times B^2 [\{4K_{A\rho}(T) + K_{B\rho}(T) + K_{B\sigma}(T)\} /4, 1 - \{4K_{A\rho}(T) + K_{B\rho}(T) + K_{B\sigma}(T)\} /2] \\ & + 8Y_{AB\rho}^2(T) T \cos^2 [\{K_{A\rho}(T) + K_{B\rho}(T)\} \pi] B^2 [K_{A\rho}(T) + K_{B\rho}(T), 1 - 2\{K_{A\rho}(T) + K_{B\rho}(T)\}] \\ & + 9Y_{B\rho\sigma}^2(T) T \cos^2 [\{9K_{B\rho}(T) + K_{B\sigma}(T)\} \pi/4] B^2 [\{9K_{B\rho}(T) + K_{B\sigma}(T)\} /4, 1 - \{9K_{B\rho}(T) + K_{B\sigma}(T)\} /2] \\ & + 36Y_{A\rho}^2(T) T \cos^2 [9K_{A\rho}(T) \pi] B^2 [9K_{A\rho}(T), 1 - 18K_{A\rho}(T)] \\ & + 36Y_{B\rho}^2(T) T \cos^2 [9K_{B\rho}(T) \pi] B^2 [9K_{B\rho}(T), 1 - 18K_{B\rho}(T)]. \end{aligned} \quad (3.22)$$

In the above formula, any perturbation which contains $\phi_{A\rho}$ or $\phi_{B\rho}$ contributes to the resistance. Among them, $Y_{AB\rho\sigma}$ has the lowest scaling dimension and dominates the resistance. In the weak-coupling limit, we have $R(T) \propto Y_{AB\rho\sigma}^2 T^{4K_{A\rho} + K_{B\sigma} + K_{B\rho} - 3}$. The actual temperature dependence is modified from this simple power law.

IV. RESULTS FOR QUARTER-FILLED BAND

The fixed points of the spin and charge correlation exponents, K_σ^* and K_ρ^* , determine the asymptotic correlation functions. Assuming a gap in the ν spectrum for $K_\nu^* = 0$, we classify the ground-state phases into a gapless state in which all perturbations are irrelevant so that the low-energy limit is regarded as a Tomonaga-Luttinger liquid (denoted by TL in the phase diagrams below), a state with only a spin gap which we call a spin-gap state (denoted by SG), a state with only a charge gap which we call a Mott insulator (denoted by MI), and a state with both spin and charge gaps which we call a spin-Peierls state (denoted by SP). When we consider three-dimensionality, the gapless (thus metallic) state does not correspond to a Tomonaga-Luttinger liquid any more so that it is simply denoted by M. The Tomonaga-Luttinger liquid has a dominant $2k_F$ SDW correlation $\sim \exp[-(K_\rho^* + 1) \ln r]$ or a dominant $4k_F$ CDW correlation $\sim \exp[-4K_\rho^* \ln r]$. The spin-gap state has a dominant $2k_F$ CDW correlation $\sim \exp[-K_\rho^* \ln r]$. The Mott insulator has a dominant $4k_F$ CDW correlation.

Usually a spin-Peierls state is described by a localized spin system since the charge gap is much larger than the spin gap. Here we call even a state with comparable magnitudes of gaps a spin-Peierls state because it is smoothly connected with the so-called spin-Peierls state. We assume that phonons are also one-dimensional for simplicity so that we do not consider the possibility for a static lattice distortion. In any case, a coupling with $2k_F$ phonons is a necessary condition here for a spin gap and thus for a spin-Peierls state because we consider repulsive electron-electron interactions only. With a coupling with three-dimensional phonons, the spin-Peierls state here would be accompanied by a static lattice distortion.

Before we use parameters for $(\text{DCNQI})_2\text{Ag}$, we first show how the electron- $4k_F$ phonon coupling and the umklapp process interfere with each other and next show how they are affected by the electron- $2k_F$ phonon coupling, large phonon frequency and nearest-neighbor repulsion. For the bare phonon dispersion, we take $\omega_{\pi/2} = \omega_\pi/\sqrt{2}$. It is noted that the quantity f appears with $Y_\rho(l)$ as a prefactor in the renormalization equations so that we fix $f = -1$ and allow Y_ρ to be negative. We do not cut off the logarithmic singularities, $\kappa = \eta = 0$, unless explicitly mentioned.

A. Coupling with $4k_F$ phonons and umklapp process

It is noted again that the perturbative expansion gives $Y_\rho = 3X_\sigma^3/8$ for the extended Hubbard model. The umklapp process is of third order with respect to electron-electron interaction, so that it is generally weak. In this and the next subsections, we vary the strength of the umklapp process to see the interference effect.

To have a charge gap, K_ρ^* must vanish so that $X_\rho(l)$ must approach $-\infty$ in the $l \rightarrow \infty$ limit. From the renormalization equation (3.3), it requires $Y_\rho(l)$ not to vanish. Then from (3.4), $K_\rho(l)$ must be smaller than $1/4$ [$X_\rho(l)$ must be smaller than -6] for large l . For the pure Hubbard model, it is known that it cannot be smaller than $1/2$. [30] Even for the extended Hubbard model with nearest-neighbor repulsion, it is at least $3/16$. [15] Such a small $K_\rho(l)$ is achieved generally for long-range repulsion. [31] The photoemission experiment [14] may indeed suggest a long-range repulsion for (DMe-DCNQI)₂Cu. In the (DCNQI)₂Ag salts, the $4k_F$ CDW is observed [9] and the lattice would be modulated. So, it is reasonable to regard electron-phonon interaction as cooperating with the umklapp process to have such a small value of $K_\rho(l)$. This is the case when the umklapp process itself is very weak because it occurs as a high-order process.

In the absence of the electron-phonon coupling, the critical value for a finite charge gap is large (Fig. 1) and beyond the scope of the perturbative regime. However, with the electron- $4k_F$ phonon coupling, it becomes smaller. For $Y_\rho > 0$ corresponding to $f = -1$, *e.g.*, for lattice modulation of the nearest-neighbor repulsion, the umklapp process is constructively interfered with the electron- $4k_F$ phonon coupling, as is expected from the renormalization-group equations. This is the reason for the negative slope of the critical value of Y_3 at $Y_\rho = 0$ in the figure. It is noted that, even for $Y_\rho < 0$ corresponding to $f = +1$, *e.g.*, for lattice modulation of the on-site repulsion, the critical value of Y_3 does not become so large. This is because $Y_\rho(l)$ changes the sign after it decreases due to the destructive interference at the initial high-energy scale. Thus, the interference is constructive at low-energy scales irrespectively of the sign of f . This situation is in contrast to the half-filled and nearly-half-filled cases, where the opening of a spin gap is sensitive to the form factor of the electron- $2k_F$ phonon coupling. [22,23]

B. Coupling with $2k_F$ phonons

The electron- $2k_F$ phonon coupling is expected to decrease $X_\rho(l)$, enhancing the tendency for a charge gap, from (3.3). However, its tendency is very weak as clearly seen from a comparison of Fig. 1 with Fig 2 and directly from Fig. 3. There is no interference of the electron- $2k_F$ phonon coupling with the umklapp process in (3.4). This indicates again how the interference effect is important to cause the metal-insulator transition.

The role of the electron- $2k_F$ phonon coupling is mainly to enhance the tendency for a spin gap. For a sufficiently large coupling, the system has a finite spin gap (Fig. 3) as expected from (3.2). Then, the $2k_F$ CDW correlation becomes dominant. Note the phase boundary between TL and SG and that between MI and SP depends considerably on the electron- $4k_F$ phonon coupling. This is due to the fact that the electron- $2k_F$ phonon coupling is affected by both of the spin and charge correlation exponents in (3.5). Meanwhile, the electron- $4k_F$ phonon coupling is affected by only the charge correlation exponent in (3.6). Even in the weak-coupling limit [$K_\sigma(l) \simeq K_\rho(l) \simeq 1$], $Y_1(l)$ is largely affected by the correlation exponents as shown in (3.5), although $Y_3(l)$ always decreases in (3.6). Thus, the opening of a spin gap is rather sensitive to the electron- $4k_F$ phonon coupling.

C. Phonon frequency and nearest-neighbor repulsion

Now we have a clear idea about how the electron-phonon couplings interfere with the electron-electron interaction and how they determine the ground-state phase. In this subsection, we show how the phase diagram depends on the phonon frequency and the relative magnitude of $|X_\rho|$ to X_σ , *i.e.*, the nearest-neighbor repulsion in terms of the extended Hubbard model. Note that $-X_\rho/X_\sigma = 1 + 4V/U$ in this model. For $V/U = 1/4$ and $1/2$, the relative magnitude of $|X_\rho|$ becomes twice and three times as large as that for the Hubbard model, respectively, so that the results can be largely affected by the nearest-neighbor repulsion strength.

The phonon frequency relative to the Fermi energy controls the energy scale of the interference. In the antiadiabatic limit, the electron-phonon coupling simply shifts the strengths of the electron-electron scattering parameters. For finite phonon frequency below the Fermi energy, the effective interaction is retarded and the interference effect becomes largest at an energy scale comparable to the phonon frequency as in the half-filled and nearly-half-filled systems. [22,23] As the phonon frequency increases, the critical coupling strength of Y_3 for opening a charge gap decreases, while that of Y_1 for opening a spin gap increases [Figs. 4(a) and (b)]. Then the Mott insulator phase occupies a wider area in the phase diagram.

As the magnitude of $|X_\rho|$ increases, the initial value of K_ρ decreases. Then the critical value of Y_3 for opening a charge gap decreases [Fig. 4(c)]. The slope is steeper for smaller phonon frequencies. Meanwhile, the Y_1 coordinate of the cross section of the phase boundaries among TL, MI, SG, and SP does not depend so much on $|X_\rho|$.

D. Phase diagram for (DCNQI)₂Ag

According to the local density functional theory [25], the band width for (DMe-DCNQI)₂Ag is about 0.9eV. Phonons due to the dimerization are observed at about 0.08eV in the infrared spectrum [32]. We use $\sqrt{2}\omega_{\pi/2} = \omega_{\pi} = 0.4E_F$. The condition for the Mott insulator phase is easily achieved because the phonon frequency relative to the Fermi energy is not small and because the nearest-neighbor repulsion relative to the on-site repulsion is not small either. [33] We show the data [27] again for completeness (Fig. 5).

The author does not know the electron-electron and electron-phonon interaction strengths, but the qualitative aspect of the present results would not change for different electron-electron interaction strengths. Since (DMe-DCNQI)₂Ag becomes a spin-Peierls state at low temperatures (in the sense that both of the spin and charge gaps open), we expect that its electron-phonon coupling strengths are in the SP phase of the figure. Note that all of the four possible phases appear in the phase diagram in the purely one-dimensional case. This is because the Tomonaga-Luttinger liquid phase is stable for weak electron-phonon couplings. We consider a cutoff in the logarithmic singularity below, where the Tomonaga-Luttinger liquid is not realized. Then some phases disappear from the phase diagram.

E. Effects of a cutoff in the logarithmic singularity

We consider three-dimensionality by cutting off the logarithmic singularity in either the particle-particle channel or the $2k_F$ particle-hole channel as explained in the previous section. The most important effect appears in the charge degrees of freedom. It is obvious from (3.3) that a cutoff in the particle-particle channel, $\eta \neq 0$, leads K_{ρ}^* to 0, while a cutoff in the $2k_F$ particle-hole channel, $\kappa \neq 0$, leads K_{ρ}^* to infinity. Therefore, a charge gap opens in the former case, while it does not open in the latter case. Then, possible phases are a Mott insulator and a spin-Peierls state in the former case (Fig 6), and a gapless metallic state and a spin-gap state in the latter case (Fig 7).

If the nesting property is maintained in the quasi-one-dimensional case, the particle-particle channel becomes less important at low energies. Then, it is reasonable that the nesting causes a finite charge gap or makes the charge gap larger. Note that the phase boundary for a finite spin gap is shifted to the right in Fig. 6, as expected from (3.2). As the cutoff increases, a transition occurs from the spin-Peierls state to the Mott insulator at zero temperature. This is consistent with the experimental results. (DMe-DCNQI)₂Ag has strong anisotropy so that it is regarded as a good one-dimensional material and it becomes an insulator below about 120 to 150K. Meanwhile, (DI-DCNQI)₂Ag has a considerable conductivity in the transverse direction and it is an insulator already at room temperature. From the activation plot, the charge gap is estimated to be 490K [10]. (DMe-DCNQI)₂Ag becomes a spin-Peierls state at about 80K so that it has a finite spin gap at zero temperature. Meanwhile, (DI-DCNQI)₂Ag becomes antiferromagnetic below 5.5K [10] so that the spin excitation spectrum is gapless. The Mott insulator in the present study is expected to become an antiferromagnetic [or spin-density-wave (SDW)] state when weak three-dimensionality is taken into account because the repulsive interaction would produce an effective antiferromagnetic coupling in the transverse direction. The above result is reminiscent of the earlier work for localized spins at half filling which showed the instability of the spin-Peierls state in quasi-one dimension against a SDW. [34]

If the nesting property is lost in the quasi-one-dimensional case, the possibility for a finite charge gap would be very strong electron correlation, which is beyond the scope of the perturbative renormalization-group approach. This possibility may not be excluded, but we can say at least whether the temperature dependence of the resistance within the present approach is qualitatively consistent with the experimental data or not. It will be done in the next subsection. The weakened tendency for a spin gap is common with both cutoffs. Note that the tendency for a spin gap is substantially suppressed here (Fig. 7, $\kappa \neq 0$) compared with the other case (Fig. 6, $\eta \neq 0$). This is reasonable in that, in the three-dimensional case free from nesting ($\kappa \neq 0$), a spin gap opens when the phonon-mediated effective attraction overcomes the repulsion, while such condition is not necessary for the spin gap in a spin-Peierls state.

F. Temperature dependence of the resistance

Our previous work [27] has shown results which are not yet converged so that we show the convergent results here. Here, temperatures are in the unit of $E_F \simeq 2400K$. When the particle-particle channel is cut off, the resistance increases and the metal-insulator transition temperature increases (Fig. 8). With a slight three-dimensional component, the resistance increases rapidly below the transition temperature. This is obtained by renormalizing both Y_{ρ} and K_{ρ} . If only Y_{ρ} is renormalized, the resistance is not so steep below the transition temperature. Including this, the overall and qualitative behavior of the resistance is indeed consistent with the experimental one for (DMe-DCNQI)₂Ag and

(DI-DCNQI)₂Ag. [10] Thus, we consider that a cutoff in the particle-particle channel imitates the effect of three-dimensionality for (DCNQI)₂Ag salts. When the $2k_F$ particle-hole channel is cut off on the other hand, the resistance decreases and the system finally becomes metallic at low temperatures (Fig. 9). This is obviously contradictory with the experimental data, as it is expected from the renormalization-group equations.

The real difference between (DMe-DCNQI)₂Ag and (DI-DCNQI)₂Ag would not be limited to the difference in the three-dimensionality. In fact, (DI-DCNQI)₂Ag has smaller bandwidth [25] so that the relative strength of electron-electron interaction would be larger than (DMe-DCNQI)₂Ag. We calculated the resistance with increasing coupling strengths and found that the behavior is similar to the case with increasing cutoffs in the particle-particle channel (not shown). However, the spin degrees of freedom is almost unaffected. Therefore, the three-dimensionality is the key to understand their differences, although the relative coupling strength is also different and contributes to the difference in the resistance.

V. RESULTS FOR COUPLED SIXTH- AND THIRD-FILLED BANDS

The ground-state phases can be classified according to the channel(s) whose excitation spectrum has a gap. When any perturbation is irrelevant and vanishes in the low-energy limit, the limit is described as a Tomonaga-Luttinger liquid without any gap. When all of the four X_ν 's diverge and both bands have spin and charge gaps, the system would be basically described as a band insulator (if the spin and charge gaps are comparable in the magnitude). It would be realized if a CDW of period 6 is formed and the Brillouin zone is folded at $\pm\pi/6$ so that both bands have a gap at the Fermi points. Then, it may be called a Peierls insulator because it can occur by the Peierls mechanism only, *i.e.*, without the help of electron correlation. The experimentally observed, insulator phase have a CDW of period 3. There are charge gaps in both bands and a spin gap in the third-filled band only. In fact, it has a long-ranged antiferromagnetic order at low temperature. Since it can not be described by a band picture, we call it a Mott insulator. In the phase diagrams below, each phase is denoted by the number of gap(s). The three important phases above, the Tomonaga-Luttinger liquid, the Mott insulator, and the Peierls insulator, are denoted by 0, 3, and 4, respectively.

There are also other phases which do not generally occupy a wide area in the phase diagrams below. They can be artifacts of the present, lowest-order renormalization-group approach if the occupied area is very narrow. The mechanism of each phase is discussed below. The phase 1 has a spin gap either in the B band (if the correlation in the A band is comparable to or stronger than that in the B band) or in the A band (if the correlation in the B band is much stronger). The former would correspond to a freely moving (unpinned) CDW of period 3. The phase 2 has spin gaps in both bands (if $y_1 \neq 0$) or charge gaps in both bands (if $y_1 = 0$). The former would correspond to a freely moving, CDW of period 6.

A. Interference between different interactions

Before looking at the numerical results, we should consider what is suggested by the equations. When the fixed point of the correlation exponent K_ν^* is zero, there is a gap in the ν channel. For that, $X_\nu(l)$ must diverge to $-\infty$ as l goes to ∞ in the corresponding equation among (3.9) – (3.12). Since the phonon propagators exponentially decrease and thus the electron-phonon interactions (y 's) are finally integrated out, the behavior of the electronic perturbations, $Y_{AB\rho\sigma}(l)$, $Y_{AB\rho}(l)$, $Y_{B\rho\sigma}(l)$, $Y_{A\rho}(l)$, and $Y_{B\rho}(l)$, is of particular interest. If some of them diverge, they make the corresponding $X_\nu(l)$ diverge to $-\infty$ in Eqs. (3.9) – (3.12). The behavior of each perturbation $Y(l)$ largely depends upon the factor multiplied by $Y(l)$ on the right-hand side of $dY(l)/dl$ [for example, $2 - \frac{1}{2}[4K_{A\rho}(l) + K_{B\sigma}(l) + K_{B\rho}(l) + X_{B\sigma}(l)]$ for $Y_{AB\rho\sigma}(l)$]. Note that, before the equations for $Y_{A\sigma}(l)$ and $Y_{B\sigma}(l)$ (not shown) are linearized to retain the spin-rotational symmetry, the factors were $2 - 2K_{A\sigma}(l)$ for $Y_{A\sigma}(l)$ and $2 - 2K_{B\sigma}(l)$ for $Y_{B\sigma}(l)$. If we neglect the interference effect, *i.e.*, if we do not consider the renormalization process where a pair of non-neutral Burgers vectors are combined to produce another Burgers vector, these factors are given by (l dependence is implicit hereafter) $2 - \frac{1}{2}(4K_{A\rho} + K_{B\sigma} + K_{B\rho})$ for $Y_{AB\rho\sigma}$, $2 - 2(K_{A\rho} + K_{B\rho})$ for $Y_{AB\rho}$, $2 - \frac{1}{2}(K_{B\sigma} + 9K_{B\rho})$ for $Y_{B\rho\sigma}$, $2 - 18K_{A\rho}$ for $Y_{A\rho}$, $2 - 18K_{B\rho}$ for $Y_{B\rho}$, $2 - 2K_{A\sigma}$ for $Y_{A\sigma}$, and $2 - 2K_{B\sigma}$ for $Y_{B\sigma}$. They are 2 – “scaling dimensions” in the field-theoretical terminology. As the scaling dimension becomes lower, the perturbation generally becomes more relevant. In the weak-coupling limit ($X_\nu \rightarrow 0$ and $K_\nu \rightarrow 1$), they are -1 for $Y_{AB\rho\sigma}$, -2 for $Y_{AB\rho}$, -3 for $Y_{B\rho\sigma}$, -16 for $Y_{A\rho}$ and $Y_{B\rho}$, and 0 for $Y_{A\sigma}$ and $Y_{B\sigma}$. The corresponding factors for the electron-phonon interactions are 0 for y_{A1} and y_{B1} and -1 for y_{A3} and y_{B3} . Namely, $Y_{A\sigma}$, $Y_{B\sigma}$, y_{A1} , and y_{B1} are marginal and the others are irrelevant in this limit. Then, a charge gap would not open in either band.

Of course, the relevance depends upon the correlation strengths. As K_ν 's become smaller, the perturbations become more relevant. More importantly, the interference effects largely affect the relevance of each perturbation in the renormalization process. The strengths of $Y_{AB\rho\sigma}$, $Y_{AB\rho}$, $Y_{B\rho\sigma}$, $Y_{A\rho}$, and $Y_{B\rho}$ are initially very small (set to be zero in the numerical calculations in the next section) because they correspond to high-order electron-electron scattering processes. However, the electron- $2\pi/3$ phonon interactions, y_{A3} , y_{B1} , and y_{B3} , interfere with one another to produce $Y_{AB\rho\sigma}$, $Y_{AB\rho}$, $Y_{B\rho\sigma}$, and the latter three then interfere with one another as well as with the electron- $2\pi/3$ phonon interactions. Once $Y_{AB\rho\sigma}$ becomes relevant and diverges, $X_{A\rho}$, $X_{B\sigma}$, and $X_{B\rho}$ diverges to $-\infty$ and gaps open in the corresponding channels. If $Y_{AB\rho}$ becomes relevant, gaps open in the channels $A\rho$ and $B\rho$. If $Y_{B\rho\sigma}$ becomes relevant, gaps open in the channels $B\sigma$ and $B\rho$. Since the scaling dimension of $Y_{AB\rho\sigma}$ is the lowest among the three, the first situation would always occur when the second or the third situation is realized. Without the electron- $4k_F$ phonon interactions, y_{A3} and y_{B3} , on the other hand, $Y_{AB\rho\sigma}$, $Y_{AB\rho}$, $Y_{B\rho\sigma}$, and $Y_{B\rho}$ remain zero (when they are initially set to be zero), so that a charge gap does not open in either band. In such a case, the situation for y_{B1} and $X_{B\sigma}$ is the same as that for y_{A1} and $X_{A\sigma}$ discussed below. In contrast to $Y_{AB\rho\sigma}$, $Y_{AB\rho}$, $Y_{B\rho\sigma}$, and $Y_{B\rho}$, the perturbation $Y_{A\rho}$ does not interfere with any other perturbation. Its scaling dimension is much higher than the others so that it would not play an important role.

It is noted that, if $Y_{AB\rho\sigma}$ or $Y_{B\rho\sigma}$ is finite (though it may be very small in the real materials), it and y_{B1} would interfere and produce y_{A3} or y_{B3} , respectively. This is also a possibility for opening charge gaps if an infinitesimal (or very small) value of y_{A3} or y_{B3} is necessary in the numerical results with a vanishing (initial value of) $Y_{AB\rho\sigma}$ or $Y_{B\rho\sigma}$ in the next section. In the present two-band system, it is essential that phonons with momenta near $2\pi/3$ contribute to y_{A1} , y_{A3} , and y_{B3} processes. In the single-band quarter-filled case, the coupling with $2k_F$ phonons interferes with the backward scattering, and the coupling with $4k_F$ phonons interferes with the umklapp process, but the two couplings do not interfere with each other (Sec. III A) in contrast to the present case.

The electron- $\pi/3$ phonon interaction y_{A1} does not interfere with another electron-phonon interaction. It only interferes with $X_{A\sigma}$. After y_{A1} is integrated out, *i.e.*, $|y_{A1}|^2 D_{\pi/3}$ vanishes at $l > l_0$ for some l_0 , $X_{A\sigma}$ follows $X_{A\sigma}(l) = [l - l_0 + X_{A\sigma}^{-1}(l_0)]^{-1}$. The fixed point is either $X_{A\sigma}^* = 0$ [$K_{A\sigma}^* = 1$] or $X_{A\sigma}^* = -\infty$ [$K_{A\sigma}^* = 0$], depending upon the sign of $X_{A\sigma}(l_0)$. In other words, when the electron- $\pi/3$ phonon interaction y_{A1} is strong enough for $X_{A\sigma}(l_0)$ to be negative, a gap opens in the channel $A\sigma$. Otherwise, the excitation spectrum of this channel is gapless. If the electron- $4k_F$ phonon interactions, y_{A3} and y_{B3} , are absent, the behavior of y_{B1} and $X_{B\sigma}$ is exactly the same as that of y_{A1} and $X_{A\sigma}$ mentioned above. Without the electron- $2k_F$ phonon interactions, y_{A1} and y_{B1} , $Y_{AB\rho\sigma}$ and $Y_{B\rho\sigma}$ remain zero (when they are initially set to be zero), so that a spin gap does not open in either band for the repulsive case, where the initial conditions for $X_{A\sigma}$ and $X_{B\sigma}$ are positive. In short, electron- $2k_F$ phonon coupling is necessary for a spin gap, while electron- $4k_F$ phonon coupling is necessary for a charge gap unless a sufficiently strong long-range interaction makes the scaling dimension of a high-order electron-electron scattering process lower than 2. This statement holds also for the single-band quarter-filled case (Sec. IV).

B. Phase diagrams

In the phase diagrams below, the charge gaps in the phases 3 and 4 are brought about by $Y_{AB\rho\sigma}$, while the spin gap in the A band in the phases 2 and 4 are brought about by y_{A1} . The spin gap in the B band is caused by either $Y_{AB\rho\sigma}$ or y_{B1} . We initially set $y_{A1} = y_{B1} = y_1$ and $y_{A3} = y_{B3} = y_3$ and vary y_1 and y_3 for several sets of $(X_{A\sigma}, X_{A\rho}, X_{B\sigma}, X_{B\rho})$, where $X_{A\rho}$ and $X_{B\rho}$ are negative. The strengths of $Y_{AB\rho\sigma}$, $Y_{AB\rho}$, $Y_{B\rho\sigma}$, $Y_{A\rho}$, and $Y_{B\rho}$ are initially (*i.e.*, at $l = -\infty$) set to be zero in the numerical calculations since they are of high order with respect to electron-electron scatterings. For the bare phonon dispersion, we take $2\omega_{\pi/3} = 2\omega_{2\pi/3}/\sqrt{3} = 0.4E_F$ as in the previous section unless explicitly mentioned.

When electron correlation is weak in both bands (Fig. 10), the phase diagram mainly consists of the phase 0 (Tomonaga-Luttinger liquid) and the phase 4 (Peierls insulator), as expected, unless only the electron- $4k_F$ phonon coupling y_3 is strong. As the electron- $2k_F$ phonon coupling y_1 increases, a spin gap opens in the B band either mainly by y_{B1} (phases $0 \rightarrow 1$) or by constructive interference of y_{B1} with y_{A3} and y_{B3} (phases $0 \rightarrow 3$). The phase 1 may be changed into the phase 3. As y_1 further increases, a spin gap opens also in the A band (phases $1 \rightarrow 2$, phases $3 \rightarrow 4$). It should be noted that the correlation strength ($X_{A\sigma}$, $X_{A\rho}$), the electron- $2k_F$ phonon coupling strength (y_{A1}), and the electron- $4k_F$ phonon coupling strength (y_{A3}) in the A band are the same as the corresponding coupling strengths in the B band in this figure, but a spin gap opens first in the B band. This is due to the constructive interference of y_{B1} with y_{A3} and y_{B3} . In fact, the critical coupling strengths for spin gaps are the same for $y_3 = 0$ and different for $y_3 \neq 0$. As y_3 increases, the difference becomes large because the critical coupling strength for a spin gap in the B band becomes small.

When electron correlation is strong in the A band (Fig. 11), a stronger electron- $2k_F$ phonon coupling y_1 is necessary

for a spin gap in the A band, as expected. If the correlation remains weak in the B band, the relation between the critical coupling strength for a spin gap in the B band and that for charge gaps is very similar to the weakly correlated case. Namely, as y_1 increases, a spin gap opens in the B band either mainly by y_{B1} (phases $0 \rightarrow 1$) or by constructive interference of y_{B1} with y_{A3} and y_{B3} (phases $0 \rightarrow 3$). Then, the phase 1 is changed into the phase 3. Finally, when y_1 overcomes the strong correlation in the A band, a spin gap opens in the A band (phases $3 \rightarrow 4$). As a consequence, the phase diagram mainly consists of the phases 0 (Tomonaga-Luttinger liquid), 3 (Mott insulator with a CDW of period 3), and 4 (Peierls insulator with a CDW of period 6). It should be noted again that the electron- $4k_F$ phonon coupling is necessary for charge gaps. On the y_1 axis ($y_3 = 0$), the possible phases are 0, 1, and 2. Therefore, the condition for the phase 3 is strong correlation in the A band, moderate electron-phonon couplings (not too strong to overcome the electron correlation in the A band), and finite electron- $4k_F$ phonon coupling though it may be small.

On the other hand, when electron correlation is strong in the B band (Fig. 12), a stronger electron- $2k_F$ phonon coupling y_1 is necessary for a spin gap in the B band, unless y_3 is strong. Meanwhile, the critical coupling strength for a spin gap in the A band remains small if the correlation remains weak in the A band. This situation does not correspond to (DCNQI)₂Cu salts because the correlation is expected to be stronger in the A band. If y_3 is small, a spin gap in the A band opens first and then the other three gaps open as y_1 increases. If y_3 is large on the other hand, the three gaps except the spin gap in the A band open first. Note the phase 1 here is different from that in the other figures in the sense that the A band has a spin gap here.

When electron correlation is strong in both bands and their strengths are the same (Fig. 13), the phase 1 disappears and the phase 2 exists only if $y_3 = 0$ (spin gaps) or if $y_1 = 0$ (charge gaps). The critical coupling strength for a spin gap in the B band is the same as that in the A band for $y_3 = 0$ and becomes smaller than the latter once $y_3 \neq 0$ as in Fig. 10. The two curves for these critical coupling strengths are shifted to the right for small y_3 , compared with Fig. 10.

So far we took $X_{A\sigma} = |X_{A\rho}|$ and $X_{B\sigma} = |X_{B\rho}|$, assuming only the on-site repulsion in electron-electron interactions. When we consider nearest-neighbor repulsion, for example, such a relation no longer holds. Recall that, in terms of the single-band extended Hubbard model, $X_{A\sigma} = (U + V)/(\pi v_F)$, $X_{A\rho} = -(U + 3V)/(\pi v_F)$ for sixth filling, and $X_{B\sigma} = (U - V)/(\pi v_F)$, $X_{B\rho} = -(U + 5V)/(\pi v_F)$ for third filling. Even for the same coupling strengths in terms of the extended Hubbard model, the scattering strengths depend on the filling factor. Neglecting the difference in the Fermi velocities for simplicity and taking the X values of the single-band extended Hubbard model for sixth and third fillings, we study the effect of the nearest-neighbor repulsion with $U/(\pi v_F) = 0.4$ and $V/(\pi v_F) = 0.1$ (Fig. 14). The resultant phase diagram is similar to Fig. 11 because $X_{A\sigma} > X_{B\sigma}$. When compared with the result for $U/(\pi v_F) = 0.4$ and $V/(\pi v_F) = 0$ (Fig. 10), the nearest-neighbor repulsion increases the critical coupling strength for a spin gap in the A band and decreases that for a spin gap in the B band, as expected from the fact that the nearest-neighbor repulsion increases $X_{A\sigma}$ and decreases $X_{B\sigma}$.

Experimentally, pressure induces the metal-insulator transition. The transition is of first order due to the third-order commensurability energy [26] and it needs three-dimensionality in phonons, which is beyond the scope of the present study. As temperature decreases, the resistance abruptly increases at the transition under pressure for (R_1R_2 -DCNQI)₂Cu with $R_1=R_2=\text{CH}_3$ or I, but above the transition temperature the resistance behaves as at ambient pressure where no transition occurs. The pressure would change the band width at least, but it hardly affects the behavior of the resistance above the transition temperature. We decrease the band width by multiplying X 's, $|y|^2$'s, and ω 's (all of which scale as the inverse of the band width) by a common factor (1.1 to 1.4) and calculated the temperature dependence of the resistance in the case of Fig. 11 with y_1 and y_3 near the boundary between the phases 0 and 3 (Fig. 15). The overall behavior of the resistance is insensitive to changes in the parameters even near the metal-insulator transition, which is qualitatively consistent with the experimental results. This is in contrast to the quarter-filled case appropriate for (DCNQI)₂Ag salts, where the correlation strength affects the behavior of the resistance rather sensitively. (Sec. IV)

VI. SUMMARY

Metal-insulator transitions and electronic phases in (DCNQI)₂M (M=Ag, Cu) salts are studied with the renormalization-group method for the one-dimensional continuum models with backward scatterings, umklapp processes and couplings with $2k_F$ and $4k_F$ phonons. These salts are in contrast to the quarter-filled (TMTTF)₂X and (TMTSF)₂X salts, where the extrinsic $4k_F$ anion potential produces the umklapp process. For the present salts with M=Ag, such a potential is absent but the electron- $4k_F$ phonon coupling interferes constructively with the umklapp process, thereby causing a metal-insulator transition. The $4k_F$ CDW is therefore a product of the cooperation of the electron-electron and electron-phonon interactions. It can be viewed as a Mott insulator in the sense that it has gapless spin excitations and it cannot be described by a band picture.

Experimentally, the physical properties of $(R_1R_2\text{-DCNQI})_2\text{Ag}$ depend upon R_1R_2 . For $R_1=R_2=\text{CH}_3$, one-dimensionality is rather good. It becomes first an insulator at about 120K and then a spin-Peierls state at 80K, opening a spin gap. Meanwhile, for $R_1=R_2=\text{I}$, electron transfer in the perpendicular direction is not negligible and electron correlation is expected to be stronger due to the narrower bandwidth. It is already an insulator at room temperature and the spin excitation spectrum remains gapless to zero temperature. In fact, it becomes antiferromagnetic below 5.5K. Such qualitative difference is explained by the present approach if the three-dimensionality is taken into account by cutting off the logarithmic singularity in the particle-particle channel. The cutoff suppresses the opening of a spin gap and enhances the charge gap. The stronger correlation for $R_1=R_2=\text{I}$ would contribute to further enhancing the charge gap. The temperature dependence of the resistance is calculated with a memory-function approximation and its behavior is consistent with the experimentally observed one.

For $\text{M}=\text{Cu}$ with coupled sixth- and third-filled bands, the Mott transition is accompanied by the formation of a CDW. In real materials, three-dimensionality would not be neglected. Reasons why we take the one-dimensional model are: a Tomonaga-Luttinger behavior is observed in the metallic phase in photoemission experiments; and the metal-insulator transition should be explained in one dimension also.

In order for gaps to open in the charge excitations in both bands and in the spin excitation in the third-filled band, the high-order backward scattering $Y_{AB\rho\sigma}$ must be relevant. Its scaling dimension is higher than 2 in the noninteracting limit. So, it may look as an irrelevant perturbation. It is not the case if the interference of the electron- $2k_F$ phonon coupling y_{B1} with the electron- $4k_F$ phonon couplings, y_{A3} and y_{B3} , is taken into account. These electron-phonon couplings interfere with one another and produce effective high-order backward and umklapp scatterings. The interference of the electron-phonon couplings and the high-order scatterings is constructive and can make $Y_{AB\rho\sigma}$ a relevant perturbation.

In order for a gap not to open in the spin excitation in the sixth-filled band, the electron correlation must be strong enough. Therefore, the condition for the experimentally observed, Mott insulator phase with a CDW of period 3, *i.e.*, with a gapless spin mode, is strong correlation in the sixth-filled, π - d hybrid band, moderate electron-phonon couplings which are not too strong to overcome the strong electron correlation in the sixth-filled band, and finite electron- $4k_F$ phonon coupling which may be small. The temperature dependence of the resistance is found to be insensitive to changes in the parameters even near the metal-insulator transition, which is again consistent with the experimentally observed one. If electron-phonon couplings were too strong, the insulator phase would be accompanied by a CDW of period 6 and have gaps in all channels.

Showing these results, we have demonstrated that the renormalization-group method reproduces the qualitative aspects of the ground-state phases and the behavior of the resistance in these quasi-one-dimensional organic materials very well.

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FIG. 1. Phase diagram for $X_\sigma = 0.4$, $X_\rho = -0.8$, $\omega_\pi = 0.1E_F$, and $Y_1 = 0$.

FIG. 2. Phase diagram for $X_\sigma = 0.4$, $X_\rho = -0.8$, $\omega_\pi = 0.1E_F$, and $Y_1 = 0.2$.

FIG. 3. Phase diagram for $X_\sigma = 0.4$, $X_\rho = -0.8$, $Y_\rho = 0.375X_\sigma^3$, and $\omega_\pi = 0.1E_F$.

FIG. 4. Y_1 and Y_3 coordinates of the cross section of the phase boundaries among TL, MI, SG, and SP, (a) as a function of ω_π/E_F for $X_\rho = -0.8$, (b) as a function of ω_π/E_F for $X_\rho = -1.2$, and (c) as a function of $|X_\rho|$ for $\omega_\pi = 0.1E_F$. The other parameters are the same as in Fig. 3.

FIG. 5. Phase diagram for $X_\sigma = 0.4$, $X_\rho = -0.8$, $Y_\rho = 0.375X_\sigma^3$, and $\omega_\pi = 0.4E_F$.

FIG. 6. Phase diagram with a cutoff in the particle-particle channel, $\eta = 0.1$. The other parameters are the same as in Fig. 5.

FIG. 7. Phase diagram with a cutoff in the particle-hole channel, $\kappa = 0.1$. The other parameters are the same as in Fig. 5.

FIG. 8. Logarithm of resistance (in arbitrary unit) as a function of temperature (in the unit of E_F) with different cutoffs in the particle-particle channel, $\eta = 0, 0.02, 0.04, 0.06, 0.08$, and 0.1 from the bottom. The parameters are $Y_1 = 0.25$, $Y_3 = 0.6$, and otherwise the same as in Fig. 5.

FIG. 9. Logarithm of resistance (in arbitrary unit) as a function of temperature (in the unit of E_F) with different cutoffs in the particle-hole channel, $\kappa = 0, 0.01, 0.02, 0.03, 0.04$, and 0.05 from the top. The parameters are $Y_1 = 0.4$, $Y_3 = 0.8$, and otherwise the same as in Fig. 5.

FIG. 10. Phase diagram for $(X_{A\sigma}, X_{A\rho}, X_{B\sigma}, X_{B\rho}) = (0.4, -0.4, 0.4, -0.4)$.

FIG. 11. Phase diagram for $(X_{A\sigma}, X_{A\rho}, X_{B\sigma}, X_{B\rho}) = (0.8, -0.8, 0.4, -0.4)$.

FIG. 12. Phase diagram for $(X_{A\sigma}, X_{A\rho}, X_{B\sigma}, X_{B\rho}) = (0.4, -0.4, 0.8, -0.8)$.

FIG. 13. Phase diagram for $(X_{A\sigma}, X_{A\rho}, X_{B\sigma}, X_{B\rho}) = (0.8, -0.8, 0.8, -0.8)$.

FIG. 14. Phase diagram for $(X_{A\sigma}, X_{A\rho}, X_{B\sigma}, X_{B\rho}) = (0.5, -0.7, 0.3, -0.9)$.

FIG. 15. Logarithm of resistance (in arbitrary unit) as a function of temperature (in the unit of E_F) for different correlation strengths. The parameters are $(X_{A\sigma}, X_{A\rho}, X_{B\sigma}, X_{B\rho}) = (0.8, -0.8, 0.4, -0.4)$, $y_1 = 0.4$, $y_3 = 0.3$, and ω 's as before for the curve at the bottom. For the other curves, the parameters X 's, $|y|^2$'s, and ω 's are 1.1, 1.2, 1.3, and 1.4 times the above values.

































